

The Effect of Impurities on Fracture and Grain Boundary Sliding in Nano-Crystalline α -Iron



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We present our current effort to characterize crack propagation in nano-crystalline α -iron, with grain sizes from 6-12 nanometers, including the effects of different defects and impurities. Our observations include multiple mechanisms such as grain nucleation, grain boundary accommodation, and grain rotation in a combination of both intragranular and intergranular fracture. Specifically, we study grain boundary sliding with and without impurities to better understand both the effects of the impurities in grain boundary mechanisms as well as the general process by which the energy is released during plastic deformation. Our work is carried out using both molecular static and molecular dynamic simulations with embedded atom potentials.

Introduction

In the last 20 years there has been extensive research in grain refinement in metals due to both the novel and increased mechanical properties exhibited. Generally speaking in conventional metals as grain size diminishes there is an increase in grain boundary density which impedes crack propagation. This in turn leads to an observed increase in fracture toughness known as the Hall-Petch relation.

However there is an observed breakdown of the Hall-Petch curve when grain sizes are below a critical diameter. Above this critical value fracture is generally governed by dislocation activity where dislocation pile-ups strengthen the boundaries (Regime I; Fig I). Once the grain size is reduced below this critical value (Regime II) dislocation emission is impeded and the mechanisms of fracture are strongly influenced by grain boundary mechanisms. A better understanding of these mechanisms, and the effect of impurities on them, are the focus of our work.

Methods

Atomistic computer simulations are utilized in order to achieve a precise image of how the crack tip is proceeding during fracture, a shortcoming of continuum models. We use both molecular static (conjugate gradient algorithm) and molecular dynamic simulations to achieve a detailed and realistic model. Both codes utilize Embedded Atom Potentials (EAM) to best reproduce the material's properties such as heat of formation and structure.

Fracture

Interpretations and Justifications

Grain Boundary Sliding

Grain boundary sliding is a process by which grains slide past each other along, or in a zone immediately adjacent to, their common boundary (Langdon and Vastava 1982). Grain boundary sliding is one of the mechanisms observed in MD simulations of deformation of nano-crystalline materials [H. Van Swygenhoven, Phys. Rev. B]

Simulated $\Sigma 5$ Tilt Boundary

Discussion of Findings

Although far from completed our work is yielding very interesting results. Our simulations show clearly an overall increase in fracture toughness due to the addition of carbon. In pure α -iron samples, crack propagation in the intergranular mode often proceeds by the coalescence of nano-voids ahead of the crack tip (Figs.III & IV). With the addition of carbon to the boundary the nano-voids do still form but at a much higher stress intensity showing a strong increase in fracture toughness. It is often seen as well that toughness increases within the grain during intragranular propagation (Fig.II & IV) which is likely due to elastic strain energy. Moreover in pure α -iron we have observed grain growth and grain boundary migration as seen in Fig. V. This seems to be inhibited by the carbon.

In figures VIII-X we have three different boundary configurations all shown in a state immediately prior to slip. In the pure $\Sigma 5$ boundary, without any impurities or defects, the boundary slides and migrates at approximately 3.3% shear deformation. In figure VIII we have the same boundary with one carbon atom shown with 8% shear deformation imposed and slip has yet to occur. This is a significant increase in sliding resistance owing to the cohesive energy of the carbon. In figure IX we have a second configuration in which 2 carbon atoms have been placed in the boundary. The addition of another carbon atom however does not add more cohesion to the boundary and it slips under a strain similar to the pure boundary. From this we infer a critical concentration present in the boundary at which the further addition of carbon begins to actually show a decrease in cohesion. Lastly, figure X shows the same boundary with a vacancy located within the interface. As seen in the figure there seems to be a decrease in cohesion of the boundary due to the presence of the vacancy as it slips at just a little more than 2% shear.